TRIM.FaTE USER'S GUIDE
MODULE 13: OPERATION OF TRIM.FaTE IN STEADY-STATE MODE[1]

Most of the initial test case applications of TRIM.FaTE have been executed in the dynamic mode, which accepts time-varying input data and generates time-series results (e.g., hourly or monthly concentrations for a 30-year time span). However, TRIM.FaTE can also be configured to run in the steady-state mode, which calculates a steady-state solution for the chemical amount in each compartment. Scenario runs in the steady-state mode have a *much* shorter run time than dynamic runs (e.g., a few minutes vs. much longer, depending on the duration of the simulation, complexity in terms of numbers of compartments, and frequency of time-varying input data). The steady-state mode is therefore useful for testing new approaches and conducting sensitivity or Monte Carlo analyses that can require numerous iterations.

A technical description of TRIM.FaTE's steady-state mode is presented in **Volume II of the TRIM.FaTE TSD, Appendix C** (EPA 2002). That appendix includes discussion on how a steady-state run should be configured, along with technical reasons for why these changes from the dynamic set-up are necessary. A summary of potential applications for the steady-state mode is also included in that appendix. The user is encouraged to review Appendix C prior to setting up and executing a steady-state run.

To run TRIM.FaTE in the steady-state mode, the user creates a project and scenario in the same way as they would for a dynamic simulation, with a few exceptions. A summary is presented here of the steps the user must complete that are *different* for a steady-state run compared with a dynamic run. Note that these steps could also be applied to create a steady-state simulation from an existing dynamic simulation.

(1) ***Ensure that no time-varying input data are used in the scenario.*** While essentially all properties may be represented by time-varying data, the following are those that most commonly are represented by time-varying data in the current libraries (the current TRIM.FaTE library name for each property is provided in brackets):

- Horizontal wind speed [*horizontalWindSpeed*];
- Vertical wind speed [*verticalWindSpeed*];
- Wind direction [*windDirection*];
- Air temperature [*AirTemperature_K*];
- Mixing height [*top*] (used to set top boundary of air volume elements);
- Rain [*Rain*];
- Indication of day/night [*isDay*];
- Indication of growing season for plants [*AllowExchange*];
- Litter fall [*LitterfallRate*];
- Current velocity of waterbody [*currentVelocity*];

[1] Descriptions of library-specific algorithms and properties presented in this module pertain to the March 2003 versions of the TRIM.FaTE library.

- Flow rate of waterbody [*BulkWaterFlowRate_Volumetric*]; and
- Flush rate of waterbody [*Flushes_per_year*].

For each time-varying property, the user must replace the time-varying input data with constant values. Users should note that, due to limitations in the algorithms in the current library, the **AllowExchange and isDay properties must be set to either "0" or "1."** For *AllowExchange*, this means that the steady-state simulation must assume that the growing season for plants is either "on" or "off." For *isDay*, this means that the steady-state simulation must assume that it is either always day or always night.

The user should also be especially careful in developing constant values for inputs such as precipitation rate, which are either "on" (non-zero) or "off" (zero) at different times. Implications of different approaches – for example, leaving "on" or "off" all the time – should be considered, and it may even be useful to perform multiple iterations with different settings.

Note that simple averaging of some time-varying properties (e.g., wind direction) may not be appropriate. It is the user's responsibility to ensure that suitable steady-state inputs have been developed for his or her application.

(2) ***Disable all links FROM groundwater compartments by setting the "enabled" property for these links to "false."*** This step is required because the transfers from ground water for many chemicals of interest are so slow that they act as virtual sinks and prevent the solver used in TRIM.FaTE from finding a steady-state solution.

(3) ***Set the value of the scenario property "simulateSteadyState" to "true."***

(4) ***Initiate simulation.*** Select "Run Scenario" from the *Run* pull-down menu in the Scenario window (or, press Control + R) to start the scenario simulation. The results will be saved to the output directory specified by the *outputDir* scenario property.

Note that there are three scenario properties related to the operation of LSODE (the differential equation solver used by TRIM.FaTE) in steady state mode. These properties and their default values (as included in the current version of the library) are:

- *SteadySimAbsoluteTolerance* (the absolute error tolerance for the linear equation solver; default value is 1.0×10^{-12});

- *SteadySimMaxSolverIterations* (the maximum number of iterations the linear equation solver should cycle through in seeking a solution before failing; default value is 10,000); and

- *SteadySimRelaxationParam* (the relaxation parameter for the Jacobi linear equation solver; default value is 1.2).

The user should not change these properties from their default values without fully considering the impacts of the changes. For information on LSODE that would be relevant to this consideration, refer to Radhakrishnan and Hindmarsh (1993).

REFERENCES

Radhakrishnan, K., and A. Hindmarsh. 1993. Description and Use of LSODE, the Livermore Solver for Ordinary Differential Equations. National Aeronautics and Space Administration, Office of Management, Science and Technical Information Program. NASA Reference Publication 1327. Lawrence Livermore National Laboratory Report UCRL-ID-113855.

U.S. EPA. 2002. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms. EPA 453/R-02-011b. Office of Air Quality Planning and Standards.

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